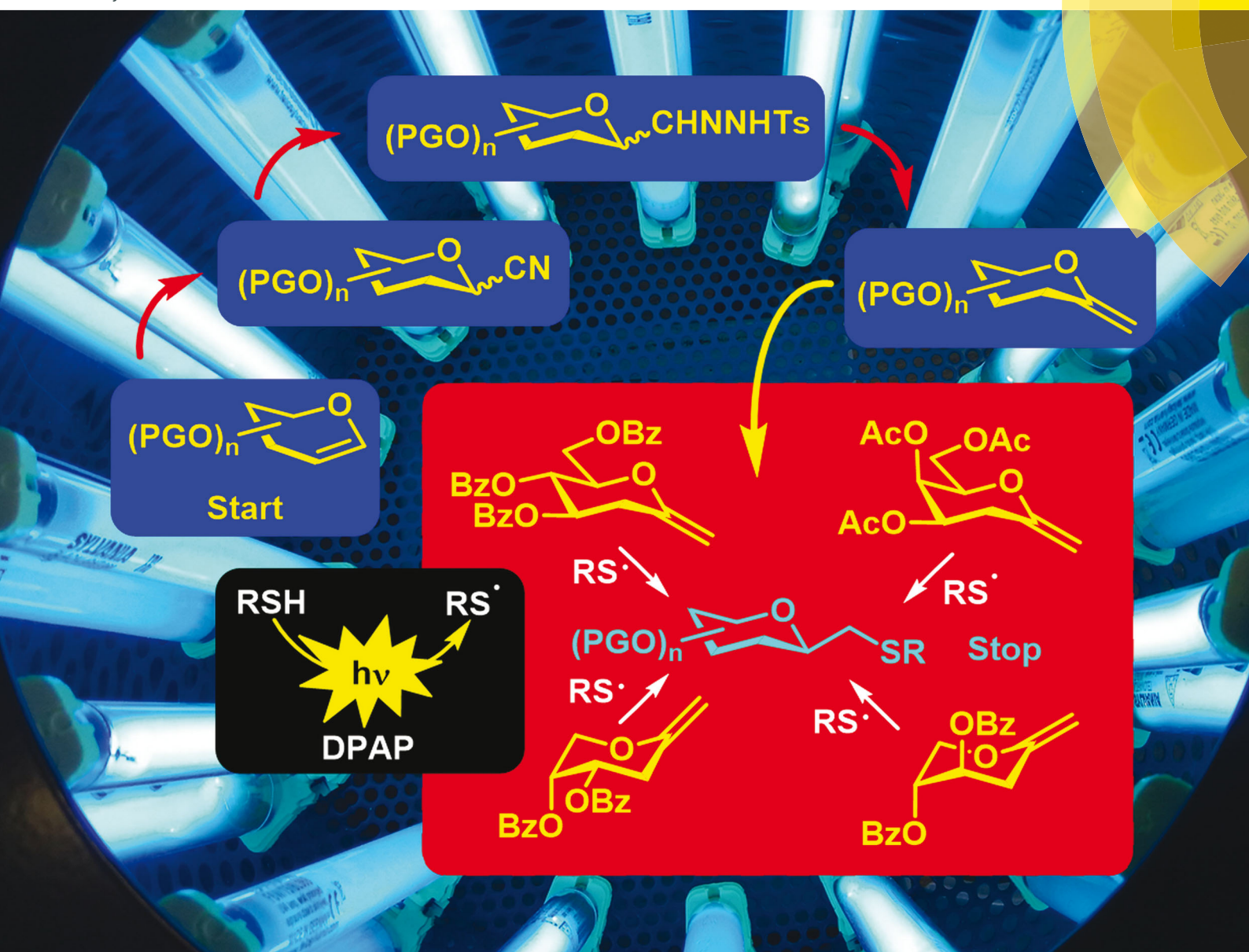


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ISSN 1144-0546



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PAPER

László Juhász, László Somsák *et al.*
Thio-click reaction of 2-deoxy-exo-glycals towards
new glycomimetics: stereoselective synthesis of
C-2-deoxy-D-glycopyranosyl compounds



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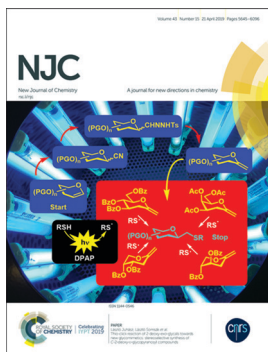
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IN THIS ISSUE

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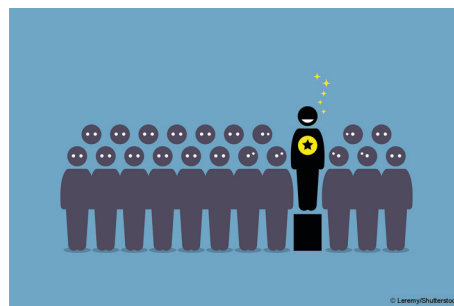
See László Juhász,
László Somsák *et al.*,
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2019, 43, 5670.

EDITORIAL

5661

Outstanding Reviewers for *New Journal of Chemistry* in 2018

We would like to take this opportunity to highlight the Outstanding Reviewers for *New Journal of Chemistry* in 2018, as selected by the editorial team for their significant contribution to the journal.



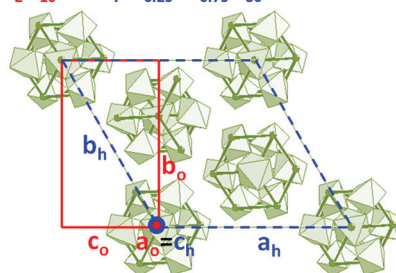
LETTERS

5662

On the crystal structures of $\text{Pr}_7\text{W}_{6.25}\text{M}_{0.75}\text{O}_{30}$ ($\text{M} = \text{Zn}, \text{Co}$) and so-called $\text{MPr}_2\text{W}_2\text{O}_{10}$ ($\text{M} = \text{Co}, \text{Mn}, \text{Cd}$)

Philippe Lacorre

Previously evidenced as exhibiting large relative permittivity, $\text{CoPr}_2\text{W}_2\text{O}_{10}$ is shown here to be $\text{Pr}_7\text{W}_{6.25}\text{Co}_{0.75}\text{O}_{30}$ with a columnar perovskite structure.



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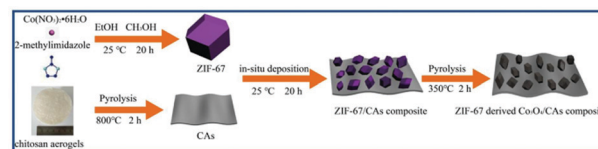
LETTERS

5666

ZIF-67 derived Co_3O_4 /carbon aerogel composite for supercapacitor electrodes

Mei-Xia Wang, Jing Zhang,* Hui-Li Fan, Ben-Xue Liu, Xi-Bin Yi and Jie-Qiang Wang*

We report carbon aerogels with a 3D hierarchical porous structure as a backbone to support nanoporous Co_3O_4 derived from ZIF-67 for supercapacitors.



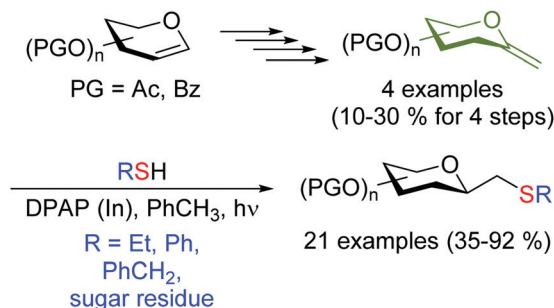
PAPERS

5670

Thio-click reaction of 2-deoxy-*exo*-glycals towards new glycomimetics: stereoselective synthesis of C-2-deoxy-D-glycopyranosyl compounds

János József, László Juhász* and László Somsák*

Photoinitiated addition of thiols to 2-deoxy-*exo*-glycals obtained from *endo*-glycals of D-*arabino*, D-*lyxo*, D-*erythro* and D-*threo* configurations resulted in highly regio- and stereoselective formation of glycosylmethyl sulfide type glycomimetics.

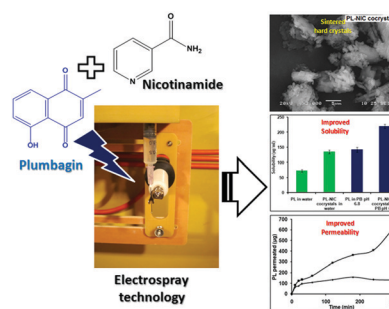


5687

Synthesis of 5-hydroxy-2-methyl-naphthalene-1,4-dione cocrystals with pyridine-3-carboxamide using electrospray technology: physicochemical characterization and *in vitro* non-everted rat intestinal absorption study

Rajalakshmi Solaimalai,* Gajanan Shinde, Abhay Dharamsi and Niraj Vyawahare

Plumbagin with nicotinamide cocrystals synthesised by electrospray technology demonstrated two-, three- and nine-fold enhancements in solubility, dissolution and permeability coefficient.

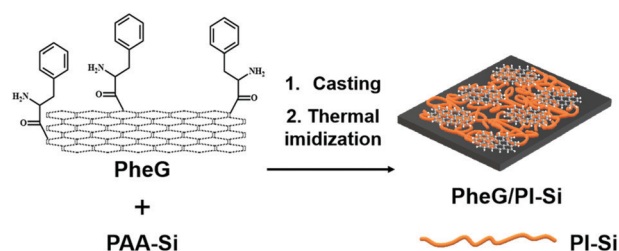


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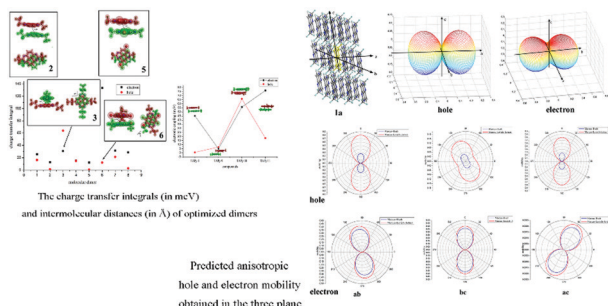
Synthesis, characterization and properties of graphene-reinforced polyimide coatings

Xing Wu, Yan Zhang, Peng Du, Zhengyu Jin, Haichao Zhao* and Liping Wang*

The prepared PheG/PI-Si composites prepared, characterized by excellent comprehensive properties, show their potential in wear resistance and lubrication applications.



5706

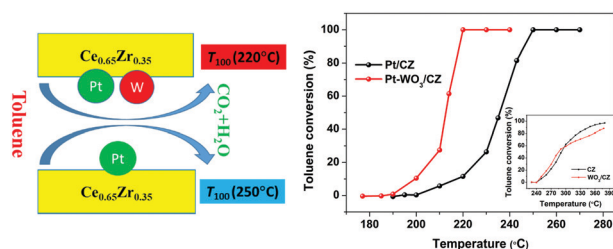


The role of electron-attracting substituents and molecular stacking motifs in the charge transport of tetraazapyrene derivatives

Ya-Rui Shi, Hui-Ling Wei and Yu-Fang Liu*

The frontier orbital energies, charge transport properties and photophysical properties of TAPy derivatives were theoretically investigated by means of DFT.

5719

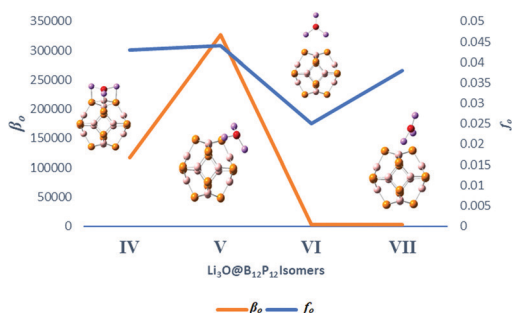


The promotion effect of tungsten on monolith Pt/Ce_{0.65}Zr_{0.35}O₂ catalysts for the catalytic oxidation of toluene

Zhongyan Hou, Xiaoying Zhou, Tao Lin,* Yaoqiang Chen, Xiaoxiao Lai, Jie Feng and Mengmeng Sun

The temperature for the complete conversion of toluene on the monolith Pt-WO₃/Ce_{0.65}Zr_{0.35}O₂ catalyst decreases by about 30 °C compared to that on Pt/Ce_{0.65}Zr_{0.35}O₂.

5727

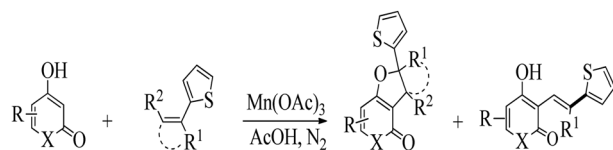


Theoretical study on a boron phosphide nanocage doped with superalkalis: novel electrides having significant nonlinear optical response

Faizan Ullah, Naveen Kosar, Khurshid Ayub, Mazhar Amjad Gilani* and Tariq Mahmood*

Three series of compounds $\text{Li}_2\text{F@B}_{12}\text{P}_{12}$, $\text{Li}_3\text{O@B}_{12}\text{P}_{12}$ and $\text{Li}_4\text{N@B}_{12}\text{P}_{12}$ are theoretically designed and investigated for their nonlinear optical response using density functional theory (DFT).

5737



Efficient syntheses and antimicrobial activities of new thiophene containing pyranone and quinolinone derivatives using manganese(III) acetate: the effect of thiophene on ring closure–opening reactions

Mehtap Özgür,* Mehmet Yılmaz, Hiroshi Nishino, Eda Çınar Avar, Hakan Dal, A. Tarık Pekel and Tuncer Hökelek

The syntheses, spectroscopic properties, and antimicrobial activities of new pyranones and quinoline-based dihydrofurans accompanied by 3-alkenyl-substituted structures were investigated.

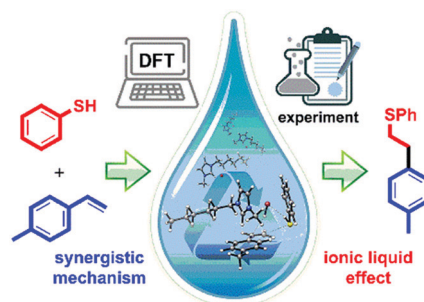
PAPERS

5752

A concerted addition mechanism in [Hmim]Br-triggered thiol–ene reactions: a typical “ionic liquid effect” revealed by DFT and experimental studies

Lin Feng, Renlong Ye, Tao Yuan, Xiao Zhang, Guo-ping Lu* and Baojing Zhou*

The $\pi^+-\pi$ and H-bond interactions between [Hmim]Br and substrates promote a special one-step addition mechanism in thiol–ene reactions.

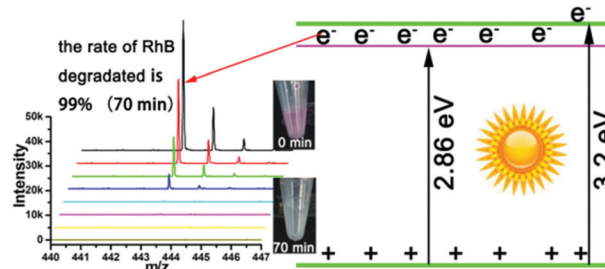


5759

Blue Ti^{3+} self-doped TiO_2 nanosheets with rich {001} facets for photocatalytic performance

Deshuai Zhen, Chan Gao, De Yang, Xingqi Zhu, Craig A. Grimes, Yu Liu* and Qingyun Cai*

The as-prepared $\text{BT}_{1.5}\text{TNs}$ exhibits superior photocatalytic performance for RhB degradation due to Ti^{3+} doping.

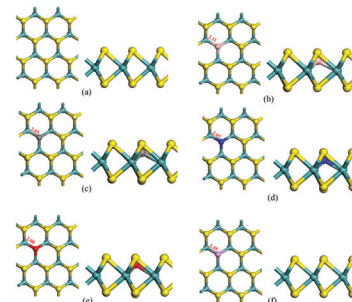


5766

Doping MoS_2 monolayer with nonmetal atoms to tune its electronic and magnetic properties, and chemical activity: a computational study

Xin Wen, Shansheng Yu,* Yongcheng Wang, Yuejie Liu,* Hongxia Wang and Jingxiang Zhao*

The introduction of heteroatom into MoS_2 nanosheet can effectively tune the electronic properties and enhance its chemical reactivity towards small molecules, thus greatly widening their applications.

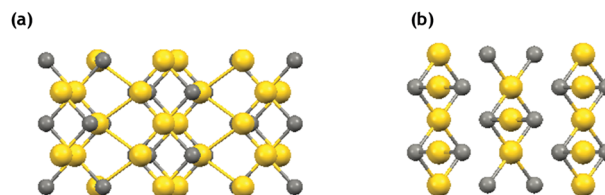


5773

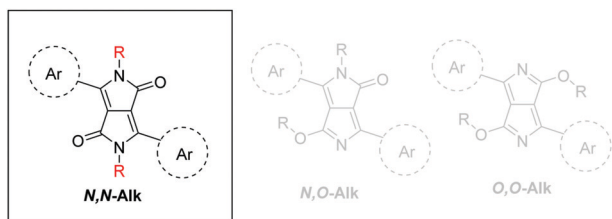
Elucidating the structural properties of gold selenide nanostructures

Lerato F. E. Machogo, Musa Mthimunya, Rudo K. Sithole, Phumlani Tetyana, Neo Phao, Grace N. Ngubeni, Mbuso Mlambo, Phumlane S. Mduli, Poslet M. Shumbula and Nosipho Moloto*

Noble transition metal chalcogenide gold selenide is a relatively unexplored layered material.



5783

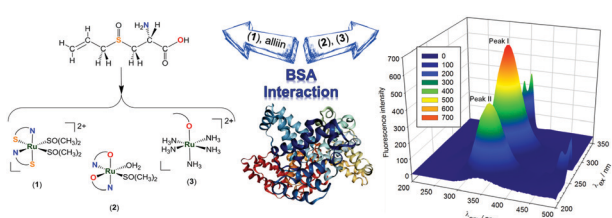


Towards more sustainable synthesis of diketopyrrolopyrroles

Flavia Pop,* Joshua Humphreys, Jesper Schwarz, Liam Brown, Ashmiani van den Berg and David B. Amabilino*

Functionalisation of diketopyrrolopyrroles with improved energy use during synthesis, ease of isolation, and yields of reactions is reported.

5791



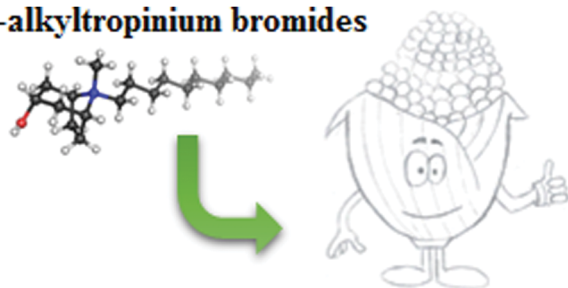
Type of complex–BSA binding forces affected by different coordination modes of alliin in novel water-soluble ruthenium complexes

Adnan Zahirović, Dijana Žilić, Sandra Kraljević Pavelić, Mirsada Hukić, Senada Muratović, Anja Harej and Emira Kahrović*

Synthesis, characterization and interaction with BSA and apo-transferrin of novel water-soluble ruthenium complexes having differently coordinated alliin (*S*-allyl-L-cysteine sulfoxide).

5805

N-alkyltropinium bromides

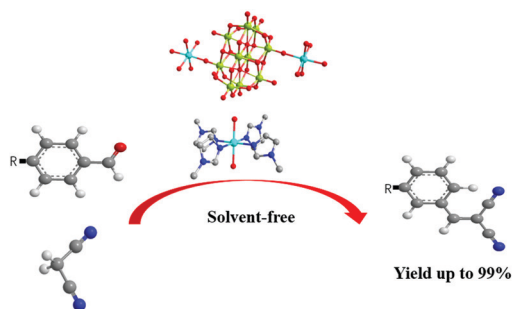


Plant growth promoting *N*-alkyltropinium bromides enhance seed germination, biomass accumulation and photosynthesis parameters of maize (*Zea mays*)

Anna Parus,* Grzegorz Framski,* Wojciech Rypniewski, Katarzyna Panasiewicz, Piotr Szulc, Kamila Myszka, Agnieszka Zgoła-Grześkowiak, Łukasz Ławniczak and Łukasz Chrzanowski

N-Alkyltropinium bromides were synthesized and characterized as novel plant-growth promoting agents.

5813



Two organic–inorganic hybrid polyoxovanadates as reusable catalysts for Knoevenagel condensation

Chunxia Li, Dandan Zhong, Xianqiang Huang,* Guodong Shen, Qiang Li, Jiyuan Du, Qianli Li, Suna Wang, Jikun Li* and Jianmin Dou*

Two novel polyoxovanadates as heterogeneous catalysts have exhibited excellent catalytic properties in the Knoevenagel condensation, especially compound **1**'s activity is basically maintained after three cycles.

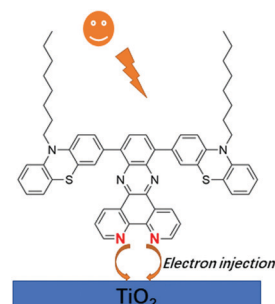
PAPERS

5820

New 2D- π -2A organic dyes with bipyridine anchoring groups for DSSCs

Hai-Lang Jia,* Zhi-Jie Peng, Bing-Quan Gong, Cheng-Yan Huang and Ming-Yun Guan

Two new 2D- π -2A-type organic dyes with bipyridine anchoring groups were synthesized and applied in dye-sensitized solar cells.

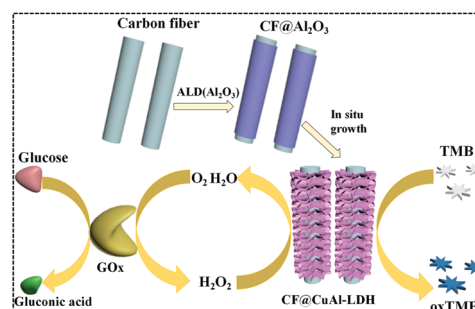


5826

Atomic layer deposition-assisted growth of CuAl LDH on carbon fiber as a peroxidase mimic for colorimetric determination of H_2O_2 and glucose

Lihong Wu, Gengping Wan, Shaohua Shi, Zhengyi He, Xuefei Xu, Yulin Tang, Chuncheng Hao and Guizhen Wang*

An atomic-layer-deposited Al_2O_3 -induced LDH growth strategy was proposed to prepare carbon fiber-supported ultrathin CuAl LDH nanosheets (CF@CuAl-LDH). The CF@CuAl-LDH exhibited superior peroxidase-like catalytic activity.

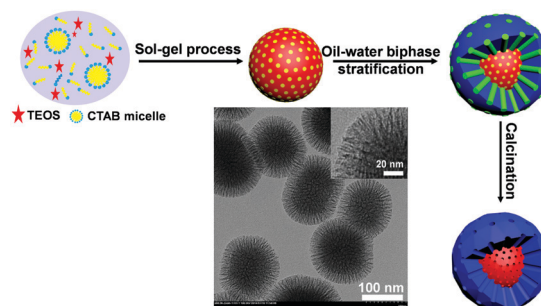


5833

Synthesis of core-shell-structured mesoporous silica nanospheres with dual-pores for biphasic catalysis

Juan Wei,* Like Zou, Yulong Li and Xiaoming Zhang*

A combination of a sol-gel process and oil-water biphasic stratification was developed to fabricate dual-pore structured MSN.

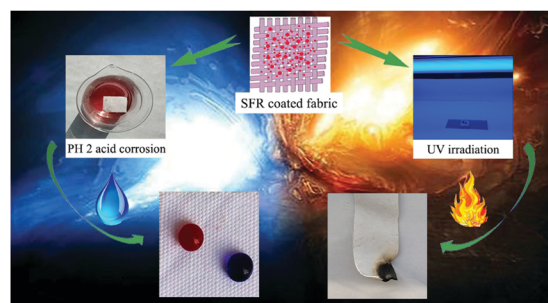


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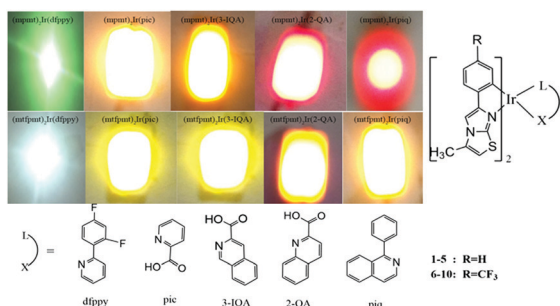
Preparation and performance testing of superhydrophobic flame retardant cotton fabric

Hongling Qin, Xuefei Li, Xiaolong Zhang and Zhiguang Guo*

A superhydrophobic flame retardant coating was fabricated using a simple method of depositing a DAP coating and a H-ZrO_2 @PDMS coating on the surface of a cotton fabric. Thermal stability tests and vertical burning tests demonstrate the excellent flame retardancy of the coating.



5849

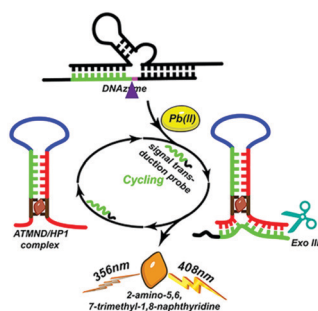


Synthesis and properties of a series of iridium complexes with imidazolo[2,1-*b*]thiazole derivatives as primary ligands

Xin-ying Yin, Zhi-yu Yang, Guo-li Huang, Jian-jian Bian, Deng-qiang Wang, Qin Wang, Ming-yu Teng,* Zheng-liang Wang* and Jie Zhang*

Ten novel phosphorescent iridium complexes based on imidazolo[2,1-*b*]thiazole derivatives as primary ligands with luminescent nearly full colors.

5857

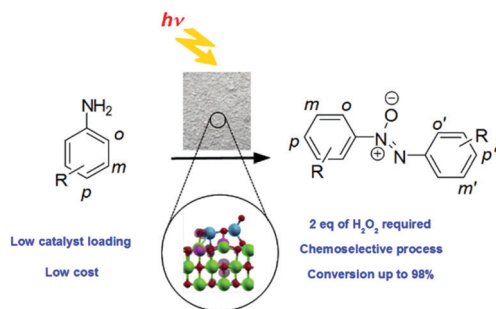


Label-free and highly sensitive fluorescence detection of lead(II) based on DNAzyme and exonuclease III-assisted cascade signal amplification

Jiafeng Pan, Qiong Li, Danhua Zhou and Junhua Chen*

A Pb^{2+} biosensor has been constructed based on Exo III-assisted cascade signal amplification using 2-amino-5,6,7-trimethyl-1,8-naphthyridine as the signal indicator.

5863

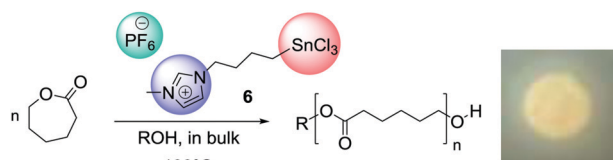


Nb_2O_5 supported on mixed oxides catalyzed oxidative and photochemical conversion of anilines to azoxybenzenes

Gustavo Senra Gonçalves De Carvalho, Luciano Honorato Chagas, Carla Grijó Fonseca, Pedro Pôssa de Castro, Antônio Carlos Sant'Ana, Alexandre Amaral Leitão and Giovanni Wilson Amarante*

Supported niobium oxide as an efficient heterogeneous catalyst for chemoselective preparation of azoxybenzenes from anilines.

5872



Organotin-bridged ionic liquid as a solvent-free, leaching-resistive catalyst for ring opening polymerization of ϵ -caprolactone

Asmaa Bouyahya, Sébastien Balieu, Redouane Beniazza, Mustapha Raihane, Abdelkrim El Kadib, Didier Le Cerf, Pascal Thébault, Géraldine Gouhier* and Mohammed Lahcini*

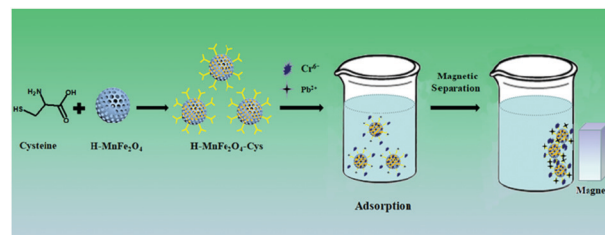
An easy synthesis provides a monoalkyltin trichloride grafted onto an ionic liquid. The catalyst paves the way to nontoxic biologically relevant materials.

5879

Functionalized hollow MnFe_2O_4 nanospheres: design, applications and mechanism for efficient adsorption of heavy metal ions

Chengzhao Jin, Guixiang Teng, Yinan Gu, Hao Cheng, ShaoPeng Fu, Chun Zhang* and Weigang Ma*

A L-cysteine functionalized magnetic hollow MnFe_2O_4 nanosphere material has been synthesised, with high magnetism, large interior cavities, and high porosity and surface activity. It has high adsorption efficiency and regenerated adsorption capacity for the removal of Cr^{6+} and Pb^{2+} in contaminated water.

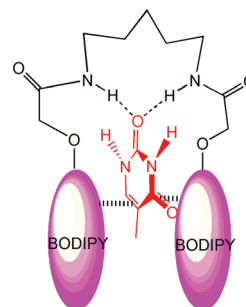


5890

A fluorescent sensor for thymine based on bis-BODIPY containing butanediamido bridges

Jiahui Bi, Xiaoyu Ji, Meiyang Guo, Hongyu Guo* and Fafu Yang*

A fluorescent sensor for thymine based on bis-BODIPY containing butanediamido bridges was prepared and applied in the sensitive detection of thymine in living cell imaging.

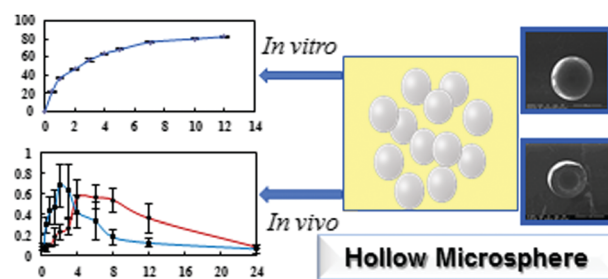


5897

Preparation and evaluation of gastro-floating hollow adhesive microspheres of carbomer/ethyl cellulose encapsulating dipyrindamole

Cheng-Yun Zhu, Jin-Yue Wang, Jin Huang, Guo-Hua Han, Yan-Yan Ji, Xiang-Rong Zhang* and Dong Liang

Gastro-floating hollow adhesive microspheres of Carbomer/ethyl cellulose encapsulating dipyrindamole were fabricated and evaluated *in vitro* and *in vivo*.

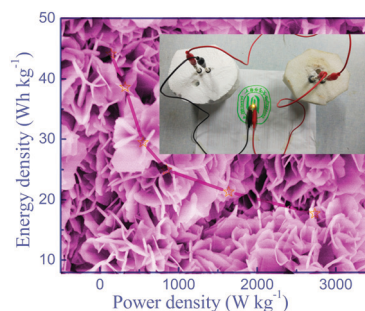


5904

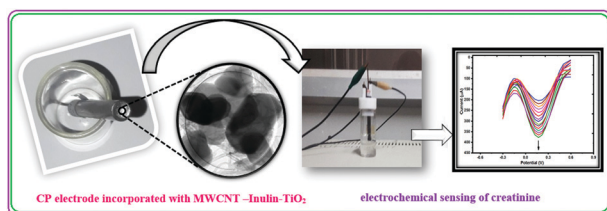
Wrapping CuCo_2S_4 arrays on nickel foam with $\text{Ni}_2(\text{CO}_3)(\text{OH})_2$ nanosheets as a high-performance faradaic electrode

Qingya Zhou, Jinping Huang,* Cuiyu Li, Zhiwei Lv, Huilin Zhu and Gang Hu

Ternary metal sulfides represent a new class of faradaic electrode material outperforming their oxide counterparts.



5914

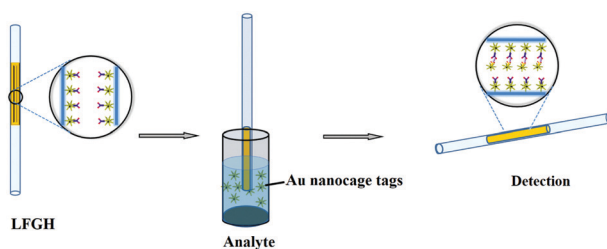


Enzyme-less sensing of the kidney dysfunction biomarker creatinine using an inulin based bio-nanocomposite

G. Jayanthi Kalaivani and S. K. Suja*

Enzyme-less electrochemical sensing of creatinine using an inulin-based bio-nanocomposite.

5925

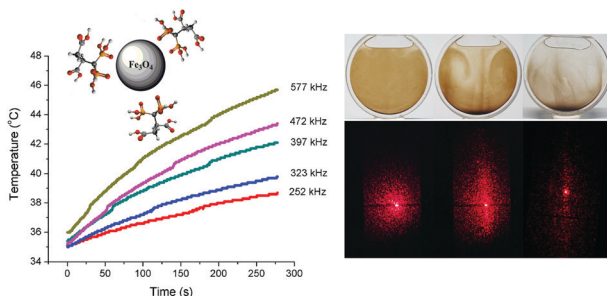


SERS based protocol using flow glass-hemostix for detection of neuron-specific enolase in blood plasma

Dawei Li, Mingfeng Yang, Hanxia Li, Leilei Mao, Ying Wang* and Baoliang Sun*

An inexpensive and disposable lateral flow glass-hemostix (FGH) has been developed as an immunoassay, in which surface-enhanced Raman scattering (SERS) is utilized for sensing signal transduction.

5932

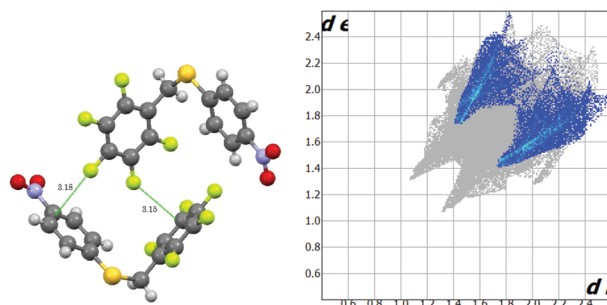


The analysis of 2,3-dicarboxypropane-1,1-diphosphonic acid-coated magnetite nanoparticles under an external magnetic field and their radiolabeling for possible theranostic applications

Marko Perić,* Magdalena Radović, Marija Mirković, Aleksandar S. Nikolić, Predrag Iskrenović, Drina Janković and Sanja Vranješ-Đurić

The advances in nanotechnology are directed towards the development of new theranostic agents based on magnetic nanoparticles that can be used for both cancer detection and treatment.

5940



Supramolecular synthons in fluorinated benzyl nitrophenyl sulfides

Maria Annunziata M. Capozzi, Angel Alvarez-Larena, Joan Francesc Piniella and Cosimo Cardellicchio*

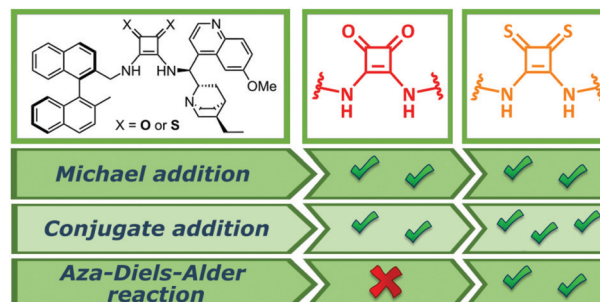
An entangled *gauche*-conformation in 4-nitrophenyl pentafluorobenzyl sulfide and its "fingerprint analysis".

5948

New enantiopure binaphthyl-cinchona thiosquaramides: synthesis and application for enantioselective organocatalysis

Sándor Nagy, Gyula Dargó, Péter Kisszékelyi, Zsuzsanna Fehér, András Simon, Júlia Barabás, Tibor Hóltzl, Béla Mátravölgyi, Levente Kárpáti, László Drahos, Péter Huszthy and József Kupai*

Binaphthyl-cinchona squaramide and thiosquaramide were applied as organocatalysts in three types of asymmetric reactions with excellent yields and enantioselectivities.

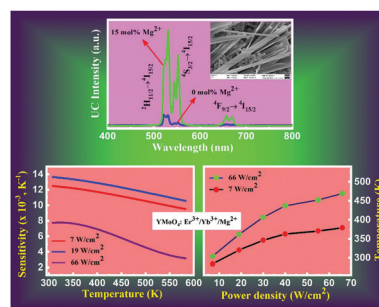


5960

Enhancing the upconversion luminescence properties of Er^{3+} – Yb^{3+} doped yttrium molybdate through Mg^{2+} incorporation: effect of laser excitation power on temperature sensing and heat generation

Shriya Sinha, Manoj Kumar Mahata* and Kaushal Kumar

Upconversion luminescence was enhanced by incorporating Mg^{2+} into Er^{3+} – Yb^{3+} -doped yttrium molybdate and the effect of laser excitation power on temperature sensing and nanoheating was investigated.

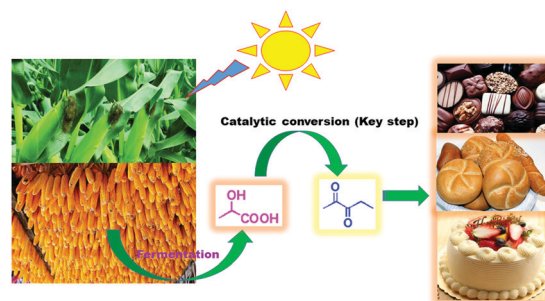


5972

An efficient and durable hierarchically porous KLA/TiPO catalyst for vapor phase condensation of lactic acid to 2,3-pentanedione

Ju Zhang, Xinli Li, Jun Pang, Weixin Zou, Congming Tang* and Lin Dong

A KLA/TPO catalyst has excellent activity due to the synergistic catalysis of Lewis acidic sites and basic sites.

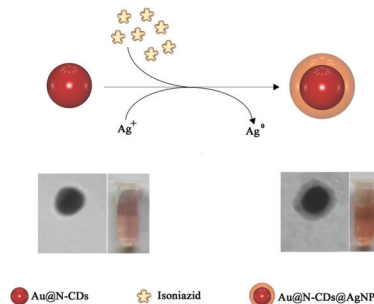


5980

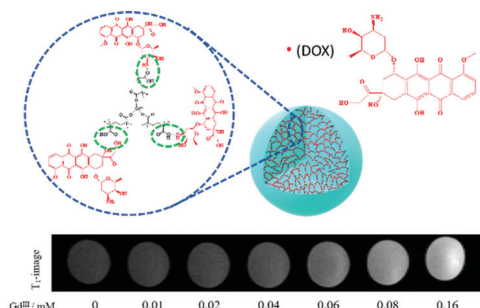
A sensitive plasmonic probe based on *in situ* growth of a Ag shell on a Au@N-CD nanocomposite for detection of isoniazid in environmental and biological samples

Tooba Hallaj* and Mohammad Amjadi

In this study, a new plasmonic probe based on the wavelength shift of the surface plasmon resonance band of a Au@N-CD nanocomposite was introduced for the determination of isoniazid.



5987

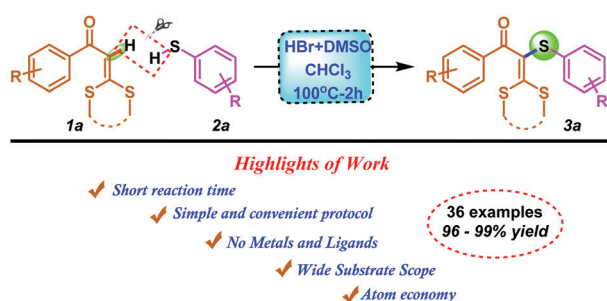


Gadolinium-containing polymer microspheres: a dual-functional theranostic agent for magnetic resonance imaging and cancer therapy

Xu Dong, Muhammad Ali Tahir, Liwu Zhang* and Christian G. Schäfer*

Preparation of poly(gadolinium methacrylate-co-methacrylic acid) copolymer microspheres with high MRI contrast efficiency and controlled anti-cancer drug loading and release capability.

5996

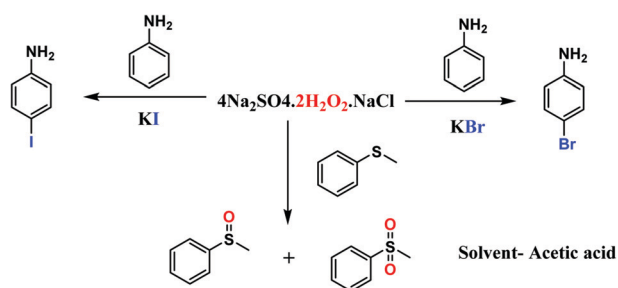


Metal free, facile sulfenylation of ketene dithioacetals catalyzed by an HBr–DMSO system

Ganesh Shivayogappa Sorabad and Mahagundappa Rachappa Maddani*

A transition metal free, efficient, sulfenylation of ketene dithioacetals catalyzed by an HBr–DMSO system is achieved. This strategy employs inexpensive and readily available HBr and DMSO to provide a direct C–H bond sulfenylation with a broad range of aryl thiols. This sulfenylated product is also transformed for the synthesis of pyrazole derivatives in excellent yield.

6001

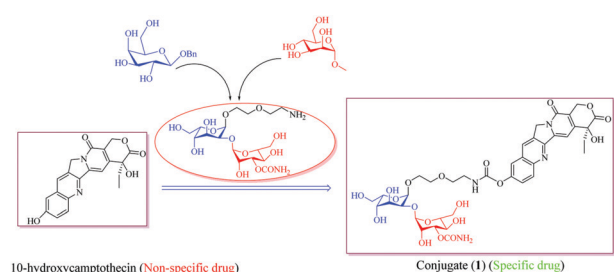


Sodium sulfate–hydrogen peroxide–sodium chloride adduct: selective protocol for the oxidative bromination, iodination and temperature dependent oxidation of sulfides to sulfoxides and sulfones

Eknath M. Gayakwad, Khushbu P. Patel and Ganapati S. Shankarling*

Sodium sulfate–hydrogen peroxide–sodium chloride adduct: selective protocols for anilines and sulfides oxidation.

6010



Multi-gram scale synthesis of a bleomycin (BLM) carbohydrate moiety: exploring the antitumor beneficial effect of BLM disaccharide attached to 10-hydroxycamptothecine (10-HCPT)

MaoLin Li, Weiping Huang, Zhilin Jiang, Yonghui Shi, Sisi Yuan, Kaishuo Fu, YongJun Chen, Li Zhou* and Wen Zhou*

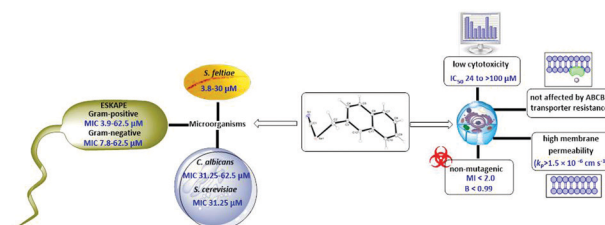
An efficient multi-gram synthesis of bleomycin disaccharide has been developed, and its conjugate with 10-HCPT displayed obvious selectivity, clearly indicating the potential of bleomycin disaccharide in solving the targeted therapy of cytotoxic drugs.

6021

Pronounced activity of aromatic selenocyanates against multidrug resistant ESKAPE bacteria

Muhammad Jawad Nasim, Karolina Witek, Annamária Kincses, Ahmad Yaman Abdin, Ewa Żesławska, Małgorzata Anna Marć, Márió Gajdács, Gabriella Spengler, Wojciech Nitek, Gniewomir Latacz, Elżbieta Karczewska, Katarzyna Kieć-Kononowicz, Jadwiga Handzlik* and Claus Jacob*

Selenocyanates demonstrate pronounced activity against bacteria of the ESKAPE family, yeast and nematodes with limited cytotoxicity against human cells.

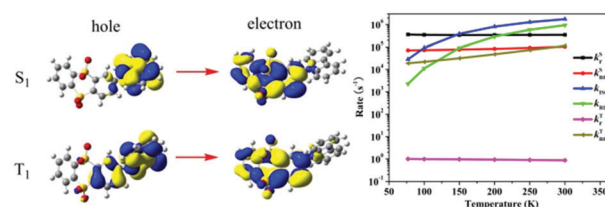


6032

A quantitative description of photoluminescence efficiency of a carbazole-based thermally activated delayed fluorescence emitter

Songyan Feng, Xugeng Guo* and Jinglai Zhang*

The present results reveal that the dominant charge transfer characteristics in the S_1 and T_1 states produce a small energy difference between the two states, and consequently an efficient reverse intersystem crossing process and a high fluorescence efficiency.

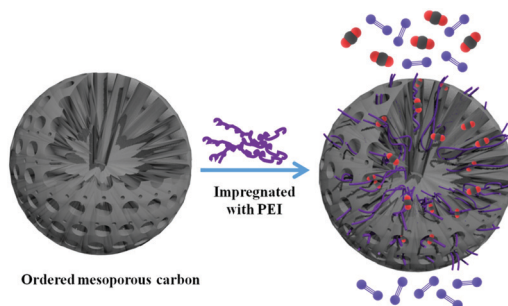


6040

Ordered mesoporous carbon with enhanced porosity to support organic amines: efficient nanocomposites for the selective capture of CO₂

Weiping Kong* and Jing Liu

Highly ordered mesoporous carbon with a much expanded porosity was impregnated with PEI to act as an efficient composite material for the highly selective capture of CO₂ from flue gas.

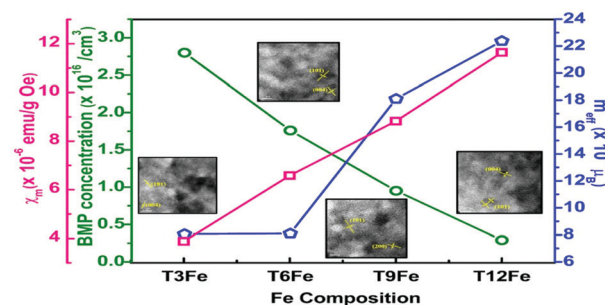


6048

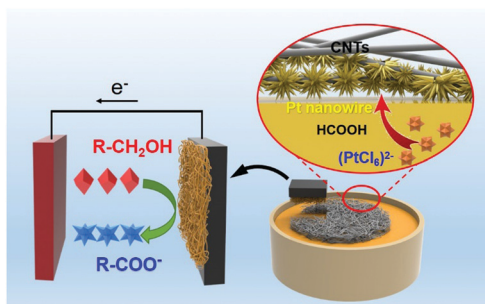
Significant reduction in the optical band-gap and defect assisted magnetic response in Fe-doped anatase TiO₂ nanocrystals as dilute magnetic semiconductors

V. R. Akshay, B. Arun, Guruprasad Mandal, Anupama Chanda and M. Vasundhara*

The nature of BMPs, whether overlapped or isolated, determines the magnetic behavior of Fe-doped TiO₂.



6063

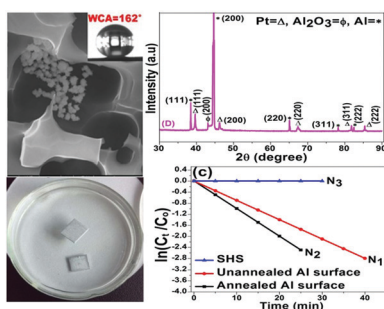


Air/water interfacial growth of Pt nanothorns anchored *in situ* on macroscopic freestanding CNT thin film for efficient methanol oxidation

Wei Zhang, Lei Zhang,* Gui Zhang, Peng Xiao, Youju Huang, Min Qiang* and Tao Chen*

One-dimensional Pt nanothorns are synthesized *via* a unique air/water interfacial process and anchored *in situ* densely on the surface of the supported CNTs film, which show efficient electrocatalytic ability for methanol oxidation.

6069

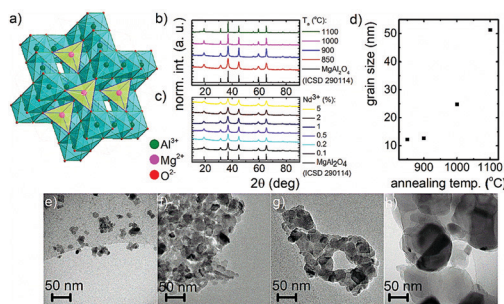


Fabrication of a Pt nanoparticle surface on an aluminum substrate to achieve excellent superhydrophobicity and catalytic activity

Noor Hassan, Shixiang Lu,* Wenguo Xu,* Ge He, Muhammad Faheem, Niaz Ahmad, Maroof Ahmad Khan and Beenish Zia Butt

A superhydrophobic Pt–Al₂O₃/Al surface with excellent application characteristics has been fabricated on an aluminium substrate by a chemical method and annealing process.

6080

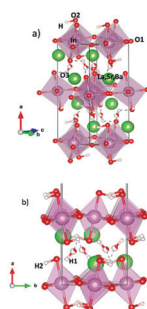


The influence of dopant concentration and grain size on the ability for temperature sensing using nanocrystalline MgAl₂O₄:Co²⁺,Nd³⁺ luminescent thermometers

A. Kobylnska, K. Kniec, K. Maciejewska and L. Marciniak*

In this work, for the first time, the ability of nanocrystalline MgAl₂O₄:Co²⁺ and MgAl₂O₄:Co²⁺,Nd³⁺ phosphors for temperature sensing was investigated in a wide temperature range.

6087



Water insertion and combined interstitial-vacancy oxygen conduction in the layered perovskites La_{1.2}Sr_{0.8-x}Ba_xInO_{4+δ}

L. Troncoso,* M. D. Arce, M. T. Fernández-Díaz, L. V. Moggi and J. A. Alonso

H₂O molecules are split within the structure with protons bonded to the axial oxygens of the InO₆ octahedra, and with OH units occupying the interstitial space.